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Dr. Mark A. Murcko  
Curriculum Vitae



### Education

1987 Ph.D. Physical Organic Chemistry, Yale University, New Haven, CT.

1984 M.S. Organic Chemistry, Yale University, New Haven, CT

1982 B.S. Summa Cum Laude, Chemistry, Fairfield University, Fairfield, CT.  
Minor: Applied Math.

### Employment History

April 1987 - May 1990: Merck Sharp & Dohme Research Laboratories, West Point, PA.  
May 1990 - present: Vertex Pharmaceuticals Incorporated, Cambridge, MA.

### Publications

30. COMPUTATIONAL METHODS TO PREDICT BINDING FREE-ENERGY IN LIGAND-RECEPTOR COMPLEXES  
AJAY; MURCKO MA  
JOURNAL OF MEDICINAL CHEMISTRY, 1995, V38, P4953-4967

29. DESIGN, SYNTHESIS AND STRUCTURE OF NON-MACROCYCLIC INHIBITORS OF FKBP12, THE MAJOR BINDING-PROTEIN FOR THE IMMUNOSUPPRESSANT FK506  
ARMISTEAD DM; BADIA MC; DEININGER DD; DUFFY JP; SAUNDERS JO; TUNG RD;  
THOMSON JA; DECENZO MT; FUTER O; LIVINGSTON DJ; MURCKO MA; YAMASHITA MM;  
NAVIA MA  
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28. COMPARATIVE X-RAY STRUCTURES OF THE MAJOR BINDING-PROTEIN FOR THE IMMUNOSUPPRESSANT FK506 (TACROLIMUS) IN UNLIGANDED FORM AND IN COMPLEX WITH FK506 AND RAPAMYCIN  
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THOMSON JA; FITZGIBBON MJ; BLACK JR; NAVIA MA  
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27. SOLVENT EFFECTS ON 1,2-DIHALOETHANE GAUCHE/TRANS RATIOS  
WIBERG KB; KEITH TA; FRISCH MJ; MURCKO M  
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26. CRYSTAL-STRUCTURE OF HIV-1 PROTEASE IN COMPLEX WITH VX-478, A POTENT AND ORALLY BIOAVAILABLE INHIBITOR OF THE ENZYME  
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JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 1995, V117, P1181-1182

25. REVERSED STEREOCHEMICAL PREFERENCE IN BINDING OF RO-31-8959 TO HIV-1 PROTEINASE - A FREE-ENERGY PERTURBATION ANALYSIS  
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24. THE SYNTHESIS AND EVALUATION OF PEPTIDYL ASPARTYL ALDEHYDES AS INHIBITORS OF ICE  
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23. STRUCTURE AND MECHANISM OF INTERLEUKIN-1-BETA CONVERTING-ENZYME  
WILSON KP; BLACK JAF; THOMSON JA; KIM EB; GRIFFITH JP; NAVIA MA; MURCKO MA; CHAMBERS SP; ALDAPE RA; RAYBUCK SA; LIVINGSTON DJ  
NATURE, 1994, V370, P270-275

22. CONFORMATIONAL-ANALYSIS OF HIV PROTEASE INHIBITORS .1. ROTATION OF THE AMIDE GROUP ADJACENT TO THE P-1(') DECAHYDROISOQUINOLINE RING-SYSTEM IN RO-31-8959 AND RELATED SYSTEMS  
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21. CONCEPTS - NEW DYNAMIC ALGORITHM FOR DE-NOVO DRUG SUGGESTION  
PEARLMAN DA; MURCKO MA  
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20. GROUPBUILD - A FRAGMENT-BASED METHOD FOR DENOVO DRUG DESIGN  
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19. GENSTAR - A METHOD FOR DENOVO DRUG DESIGN  
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JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN, 1993, V7, P23-43

18. ABINITIO MOLECULAR-ORBITAL CONFORMATIONAL-ANALYSIS OF PROTOTYPICAL ORGANIC-SYSTEMS .1. ETHYLENE-GLYCOL AND 1,2-DIMETHOXYETHANE  
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17. CHARGED SURFACE RESIDUES OF FKBP12 PARTICIPATE IN FORMATION OF THE FKBP12-FK506-CALCINEURIN COMPLEX  
ALDAPE RA; FUTER O; DECENZO MT; JARRETT BP; MURCKO MA; LIVINGSTON DJ  
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16. CDNA-ENCODING MURINE FKS06-BINDING PROTEIN (FKBP) - NUCLEOTIDE AND DEDUCED AMINO-ACID-SEQUENCES  
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15. NEW ISOMERIC CLASSES OF TOPICALLY ACTIVE OCULAR HYPOTENSIVE CARBONIC-ANHYDRASE INHIBITORS - 5-SUBSTITUTED THIENO[2,3-B]THIOPHENE-2-SULFONAMIDES AND 5-SUBSTITUTED THIENO[3,2-B]THIOPHENE-2-SULFONAMIDES  
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14. INHIBITION OF CARBONIC-ANHYDRASE  
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13. THE RESPONSE OF ELECTRONS TO STRUCTURAL-CHANGES  
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12. ORIGIN OF THE GAUCHE EFFECT IN SUBSTITUTED ETHANES AND ETHENES  
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11. THIENOTHIOPYRAN-2-SULFONAMIDES - NOVEL TOPICALLY ACTIVE CARBONIC-ANHYDRASE INHIBITORS FOR THE TREATMENT OF GLAUCOMA  
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10. ROTATIONAL BARRIERS .4. DIMETHOXYMETHANE - THE ANOMERIC EFFECT REVISITED  
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9. ROTATIONAL BARRIERS .2. ENERGIES OF ALKANE ROTAMERS - AN EXAMINATION OF GAUCHE INTERACTIONS  
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8. BOND BENDING AND HYBRIDIZATION  
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7. EVIDENCE FOR THE DIRECT INVOLVEMENT OF THE RHINOVIRUS CANYON IN RECEPTOR-BINDING  
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6. BARRIERS TO ROTATION ADJACENT TO DOUBLE-BONDS .4. EFFECT OF BASIS SET ON STRUCTURES, AND OF ELECTRON CORRELATION ON RELATIVE ENERGIES  
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5. ROTATIONAL BARRIERS .3. 2-HALOETHANOLS  
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3. NONBONDED INTERACTIONS .1. ANISOTROPIC HYDROGEN-HYDROGEN INTERACTIONS  
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1. ENTHALPIES OF HYDRATION OF ALKENES .3. CYCLOALKENES  
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